

Analyzing Parallel Program Performance using HPCToolkit

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<http://hpctoolkit.org>



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Challenges for Computational Scientists

- **Rapidly evolving platforms and applications**
 - **architecture**
 - rapidly changing designs for compute nodes
 - significant architectural diversity
 - multicore, manycore, accelerators
 - increasing parallelism within nodes
 - **applications**
 - exploit threaded parallelism in addition to MPI
 - leverage vector parallelism
 - augment computational capabilities
- **Computational scientists need to**
 - adapt codes to changes in emerging architectures
 - improve code scalability within and across nodes
 - assess weaknesses in algorithms and their implementations

Performance tools can play an important role as a guide

Performance Analysis Challenges

- Complex node architectures are hard to use efficiently
 - multi-level parallelism: multiple cores, ILP, SIMD, accelerators
 - multi-level memory hierarchy
 - result: gap between typical and peak performance is huge
- Complex applications present challenges
 - measurement and analysis
 - understanding behaviors and tuning performance
- Supercomputer platforms compound the complexity
 - unique hardware & microkernel-based operating systems
 - multifaceted performance concerns
 - computation
 - data movement
 - communication
 - I/O

What Users Want

- Multi-platform, programming model independent tools
- Accurate measurement of complex parallel codes
 - large, multi-lingual programs
 - (heterogeneous) parallelism within and across nodes
 - optimized code: loop optimization, templates, inlining
 - binary-only libraries, sometimes partially stripped
 - complex execution environments
 - dynamic binaries on clusters; static binaries on supercomputers
 - batch jobs
- Effective performance analysis
 - insightful analysis that pinpoints and explains problems
 - correlate measurements with code for actionable results
 - support analysis at the desired level
 - intuitive enough for application scientists and engineers
 - detailed enough for library developers and compiler writers
- Scalable to petascale and beyond

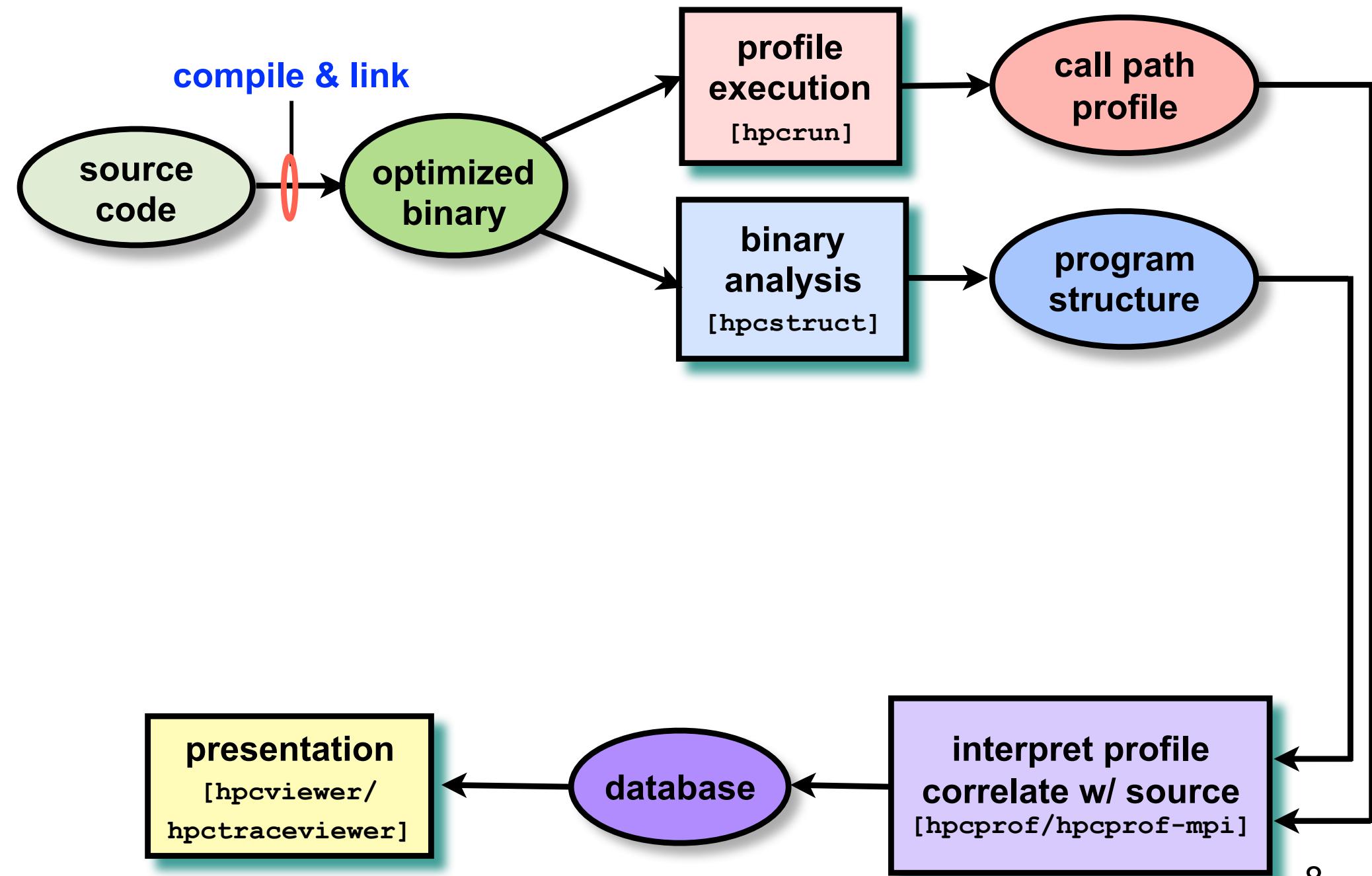
Outline

- Overview of Rice's HPCToolkit
- Pinpointing scalability bottlenecks
 - scalability bottlenecks on large-scale parallel systems
 - scaling on multicore processors
- Understanding temporal behavior
- Assessing process variability
- Understanding threading performance
 - blame shifting
- Today and the future

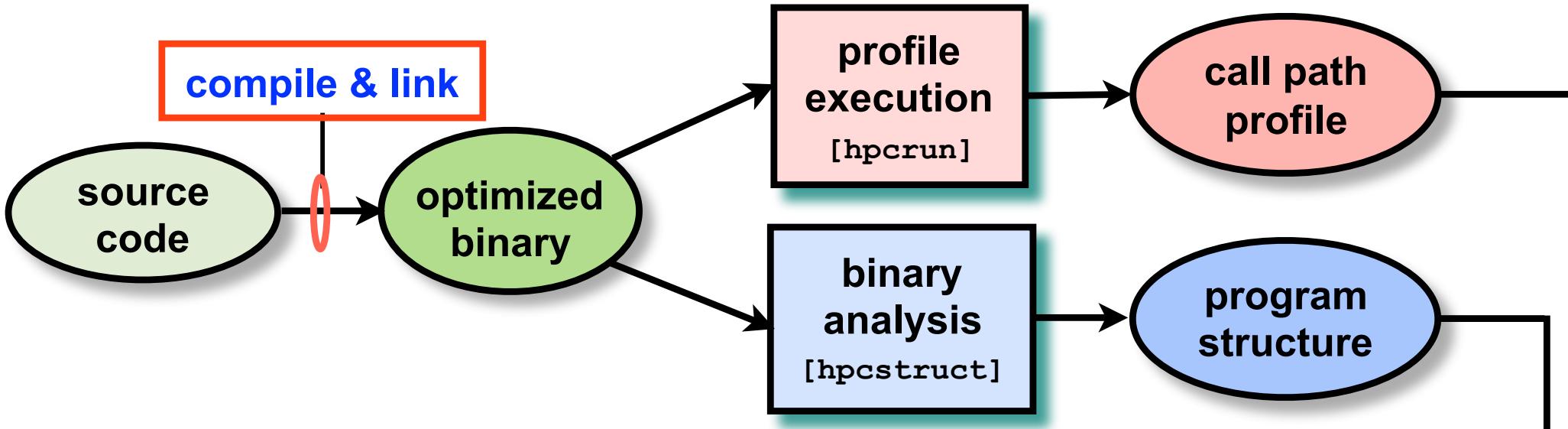
Rice University's HPC Toolkit

- Employs binary-level measurement and analysis
 - observe fully optimized, dynamically linked executions
 - support multi-lingual codes with external binary-only libraries
- Uses sampling-based measurement (avoid instrumentation)
 - controllable overhead
 - minimize systematic error and avoid blind spots
 - enable data collection for large-scale parallelism
- Collects and correlates multiple derived performance metrics
 - diagnosis often requires more than one species of metric
- Associates metrics with both static and dynamic context
 - loop nests, procedures, inlined code, calling context
- Supports top-down performance analysis
 - identify costs of interest and drill down to causes
 - up and down call chains
 - over time

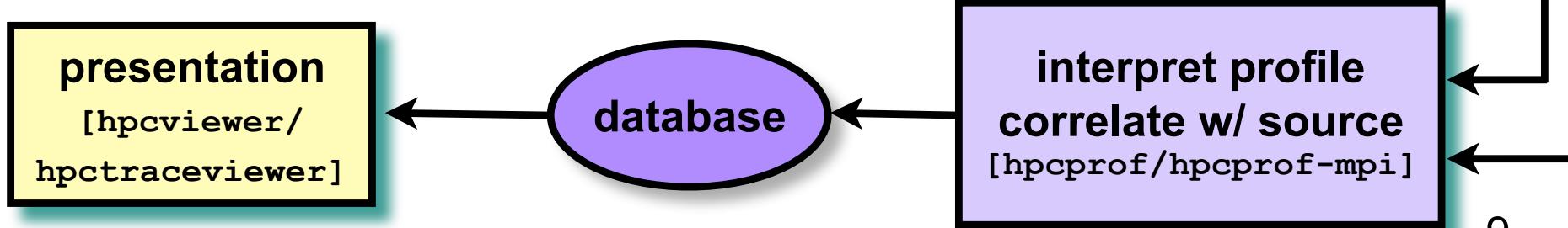
HPCToolkit Workflow



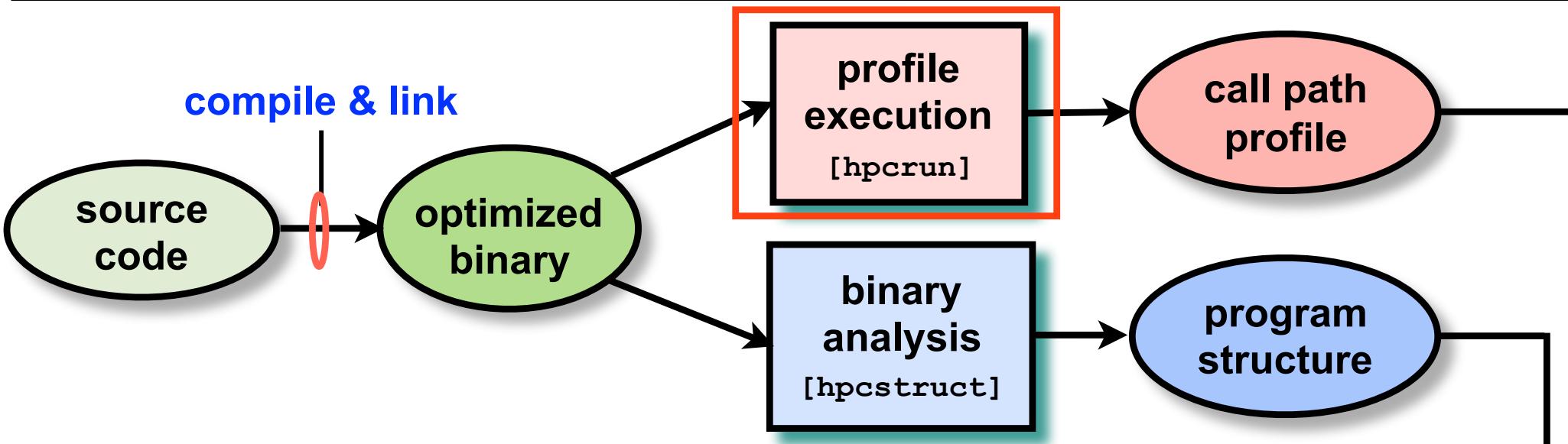
HPCToolkit Workflow



- For dynamically-linked executables, e.g., Linux clusters
 - compile and link as you usually do: nothing special needed
- For statically-linked executables, e.g., Cray, Blue Gene
 - add monitoring by using `hpmlink` as prefix to your link line
 - uses “linker wrapping” to catch “control” operations process and thread creation, finalization, signals, ...

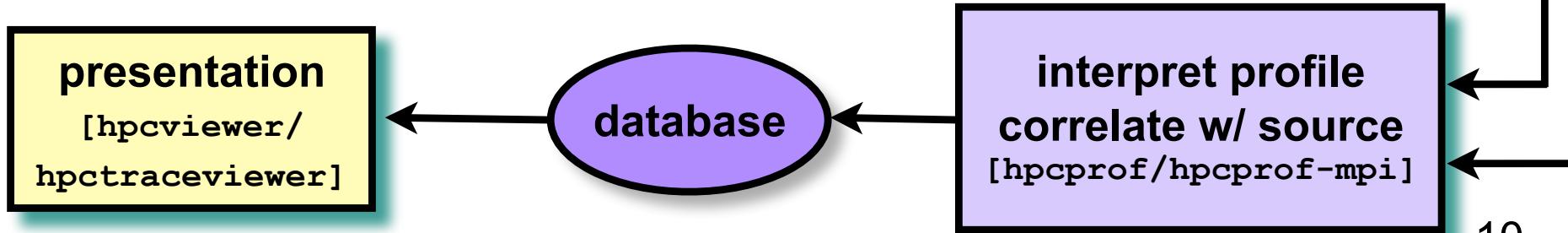


HPCToolkit Workflow



Measure execution unobtrusively

- launch optimized application binaries
 - dynamically-linked: launch with `hpcrun`, arguments control monitoring
 - statically-linked: environment variables control monitoring
- collect statistical call path profiles of events of interest



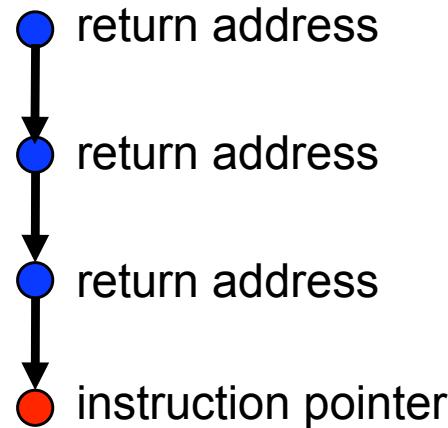
Call Path Profiling

Measure and attribute costs in context

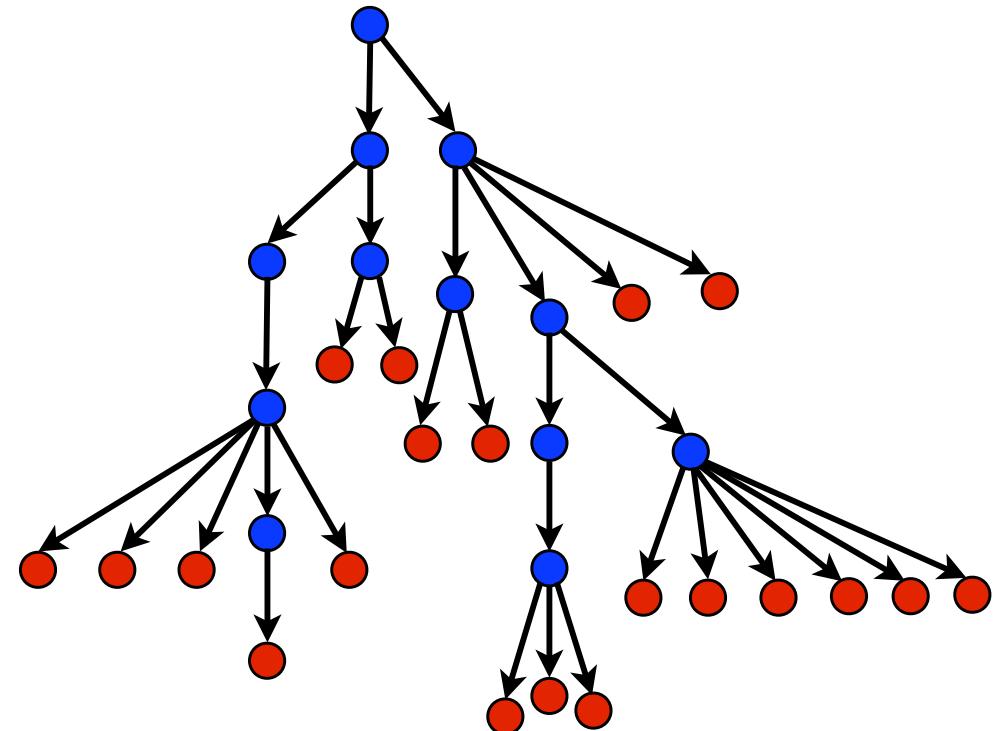
sample timer or hardware counter overflows

gather calling context using stack unwinding

Call path sample

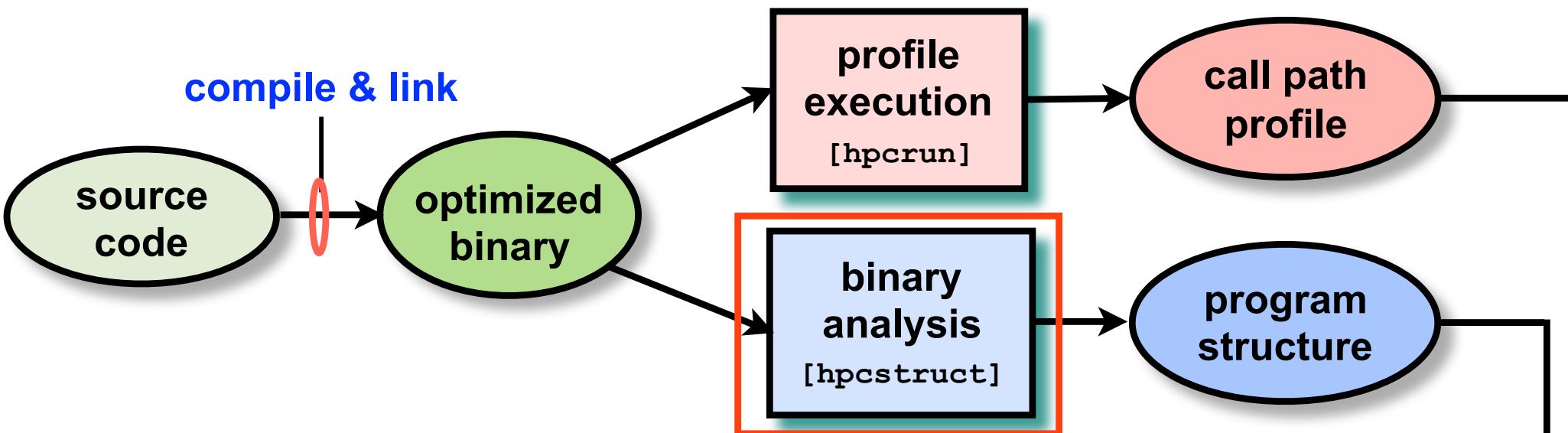


Calling context tree

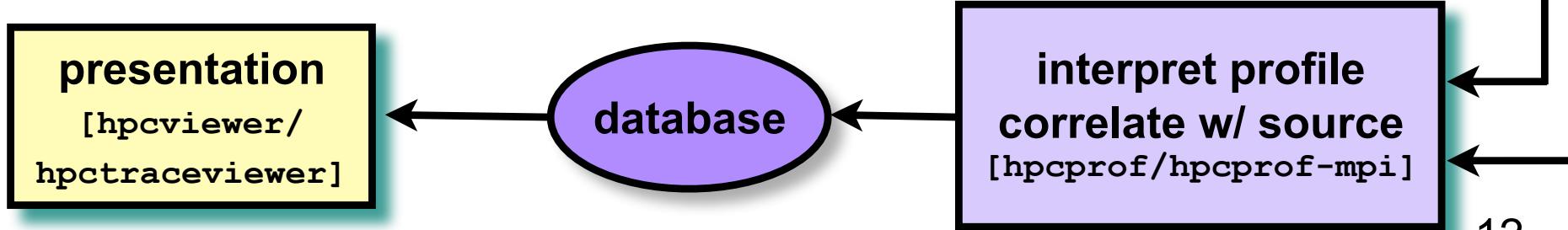


Overhead proportional to sampling frequency...
...not call frequency

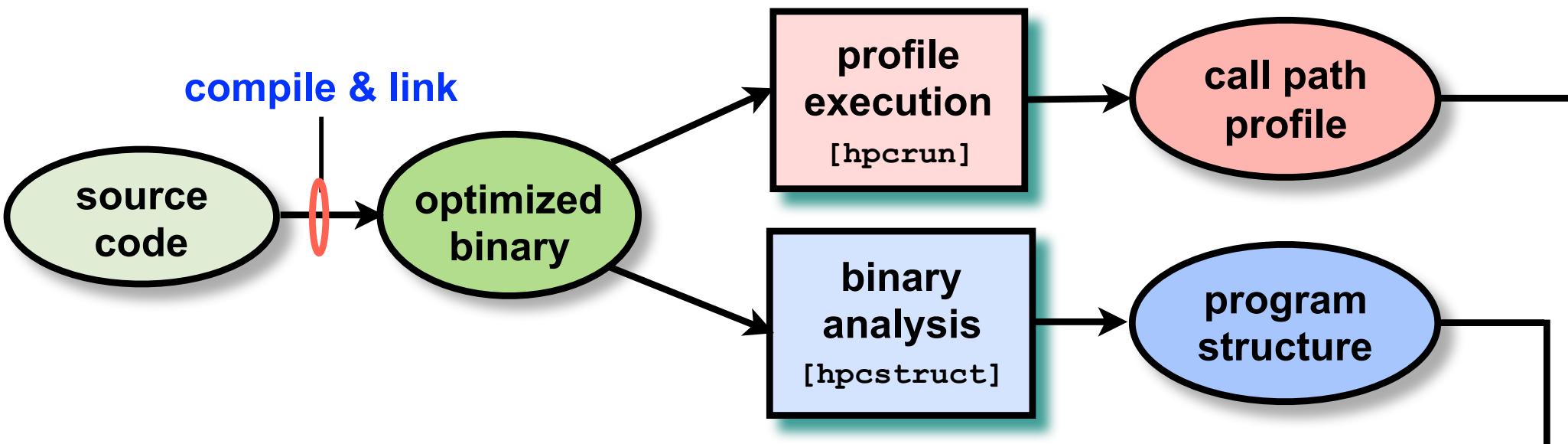
HPCToolkit Workflow



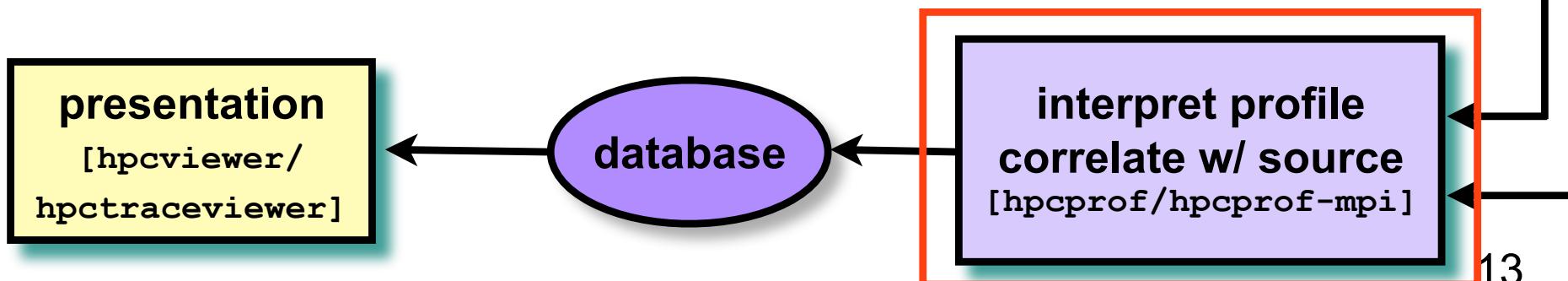
- Analyze binary with **hpcstruct**: recover program structure
 - analyze machine code, line map, debugging information
 - extract loop nests & identify inlined procedures
 - map transformed loops and procedures to source



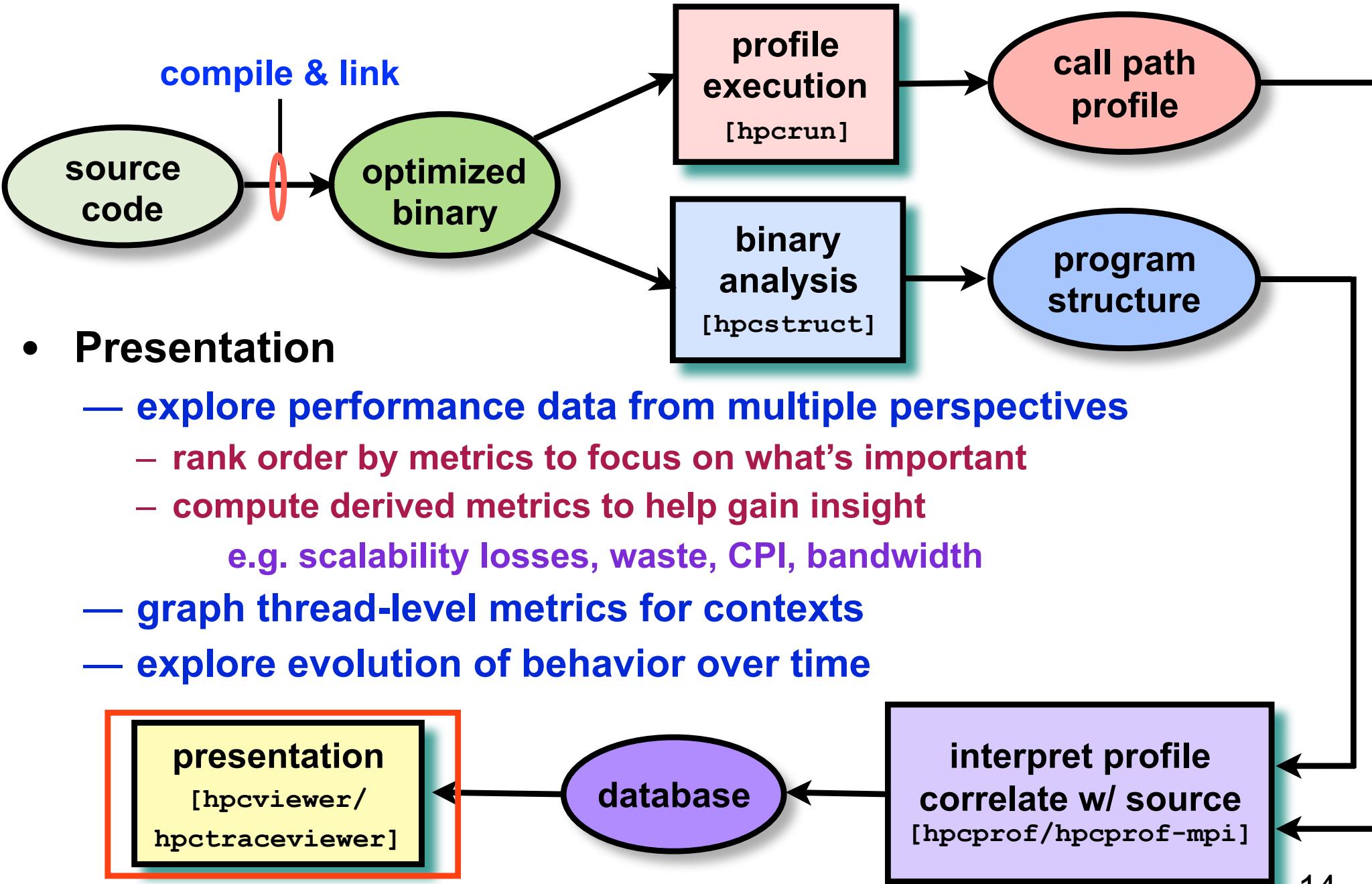
HPCToolkit Workflow



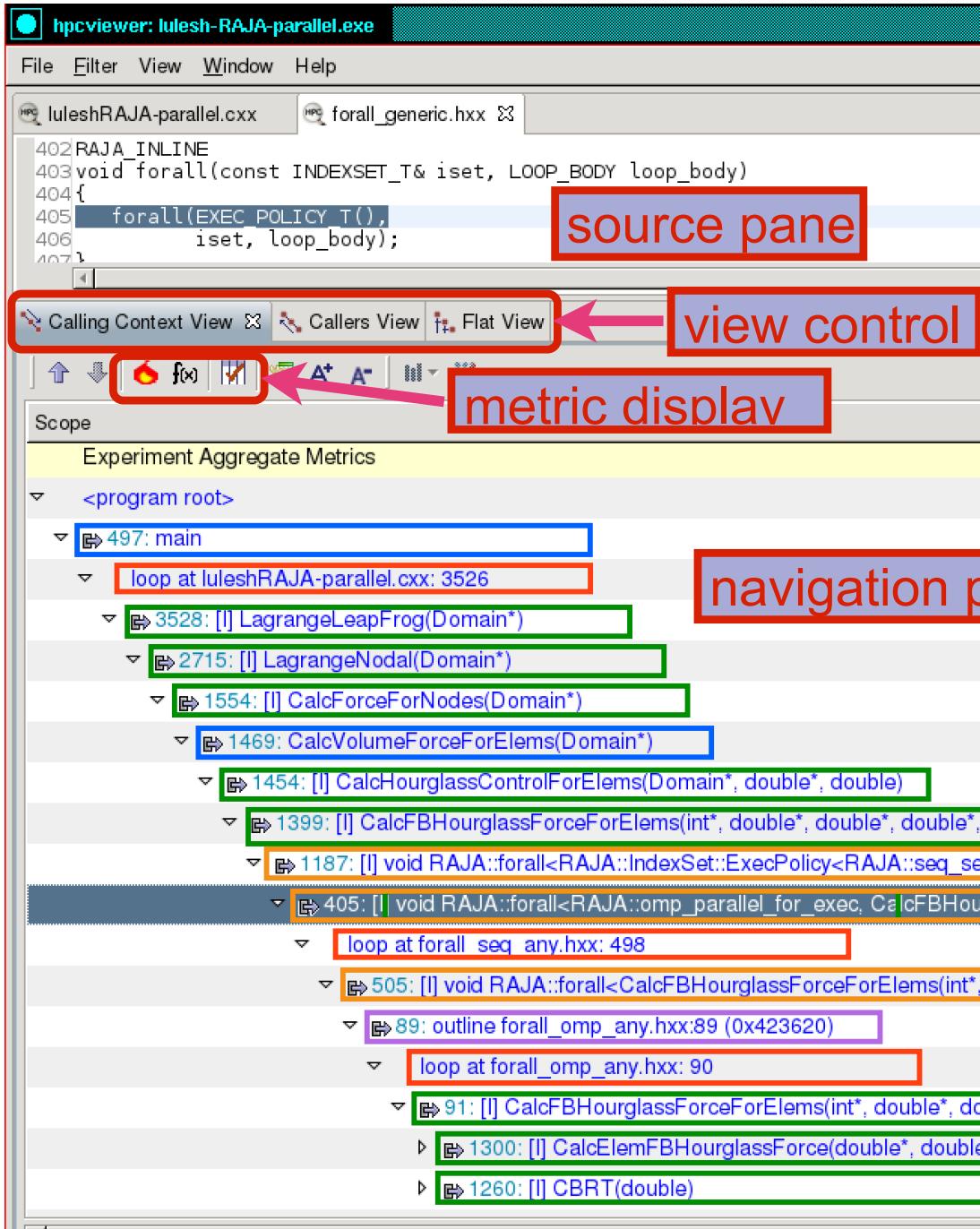
- **Combine multiple profiles**
 - **multiple threads; multiple processes; multiple executions**
- **Correlate metrics to static & dynamic program structure**



HPCToolkit Workflow

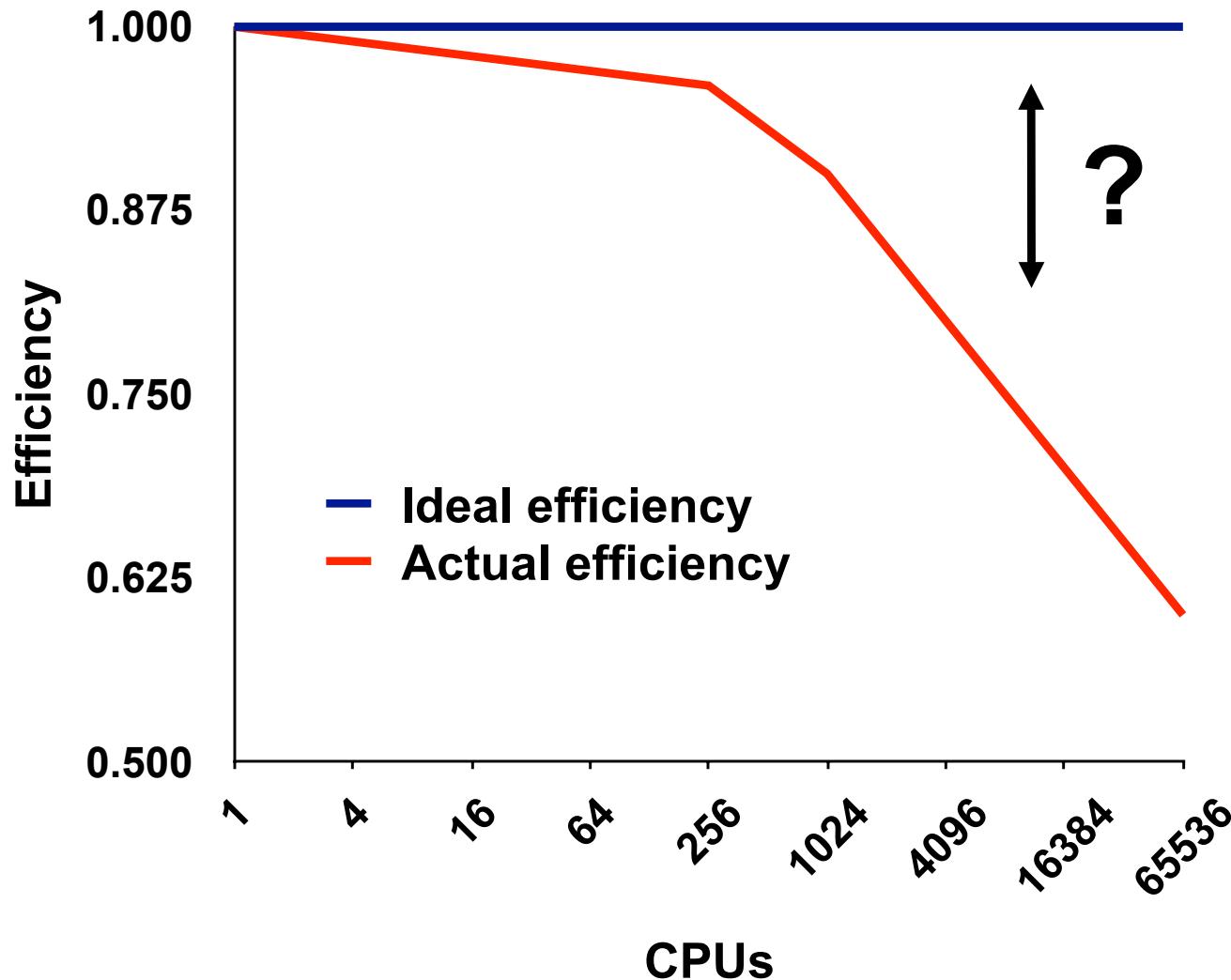


Code-centric Analysis with hpcviewer



- function calls in full context
- inlined procedures
- inlined templates
- outlined OpenMP loops
- loops

The Problem of Scaling



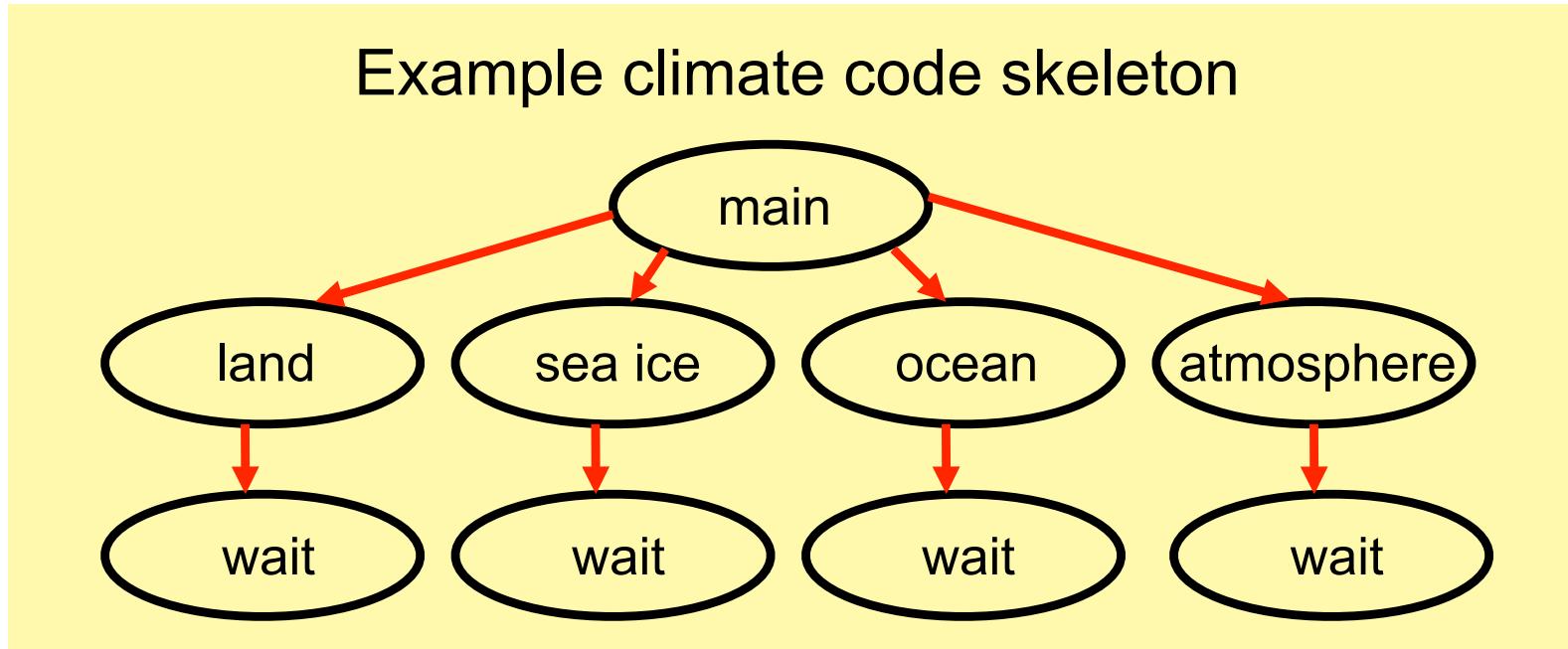
Note: higher is better

Goal: Automatic Scalability Analysis

- Pinpoint scalability bottlenecks
- Guide user to problems
- Quantify the magnitude of each problem
- Diagnose the nature of the problem

Challenges for Pinpointing Scalability Bottlenecks

- Parallel applications
 - modern software uses layers of libraries
 - performance is often context dependent

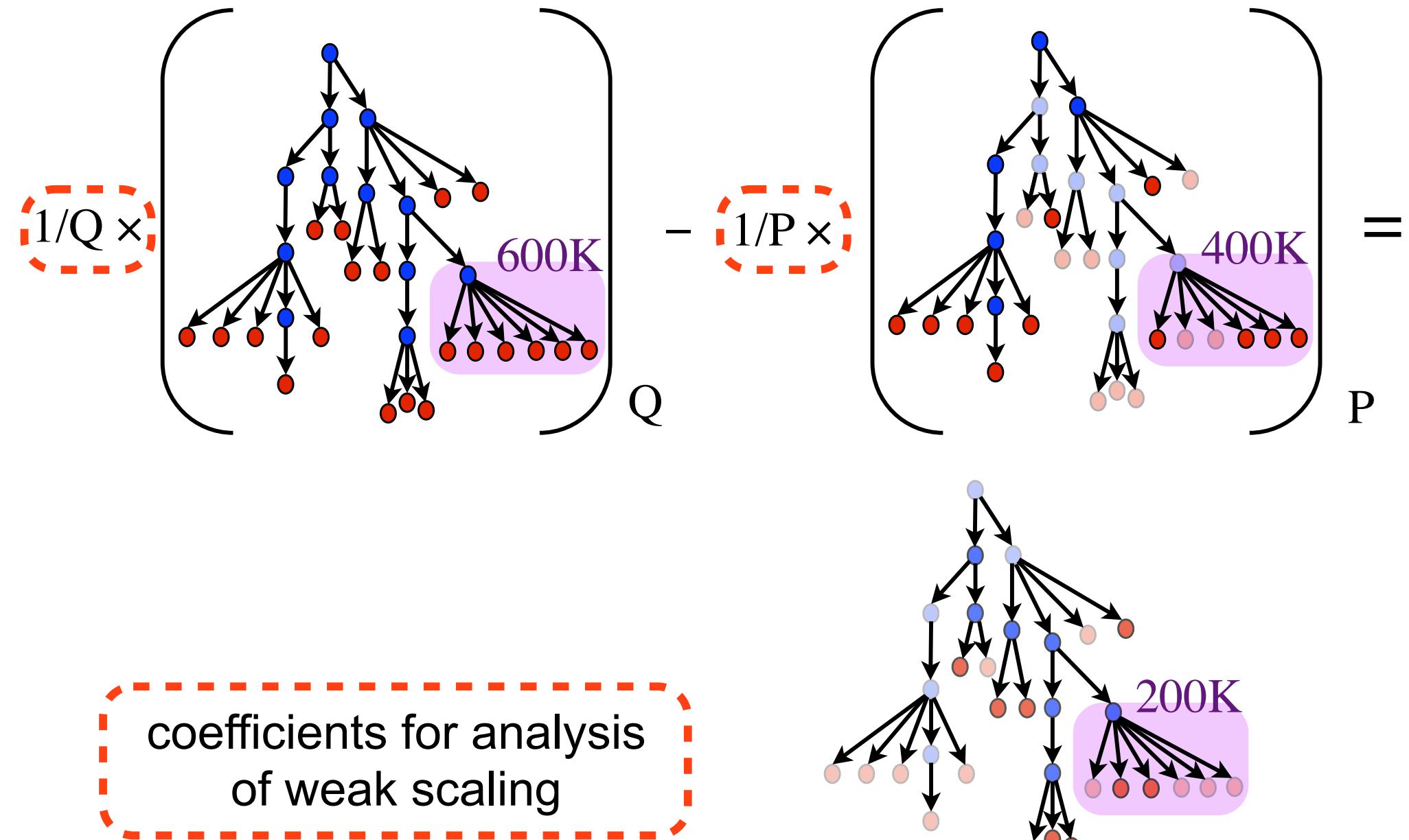


- Monitoring
 - bottleneck nature: computation, data movement, synchronization?
 - 2 pragmatic constraints
 - acceptable data volume
 - low perturbation for use in production runs

Performance Analysis with Expectations

- You have performance expectations for your parallel code
 - strong scaling: linear speedup
 - weak scaling: constant execution time
- Put your expectations to work
 - measure performance under different conditions
 - e.g. different levels of parallelism or different inputs
 - express your expectations as an equation
 - compute the deviation from expectations for each calling context
 - for both inclusive and exclusive costs
 - correlate the metrics with the source code
 - explore the annotated call tree interactively

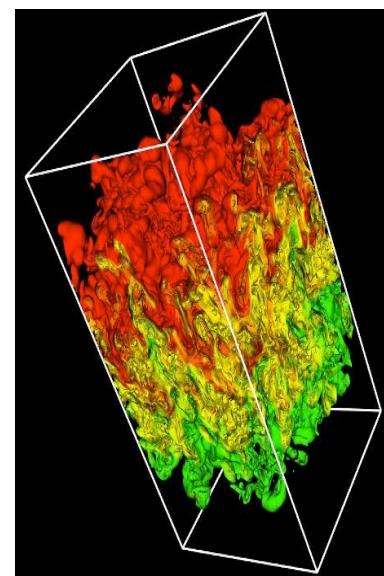
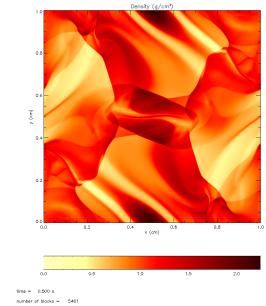
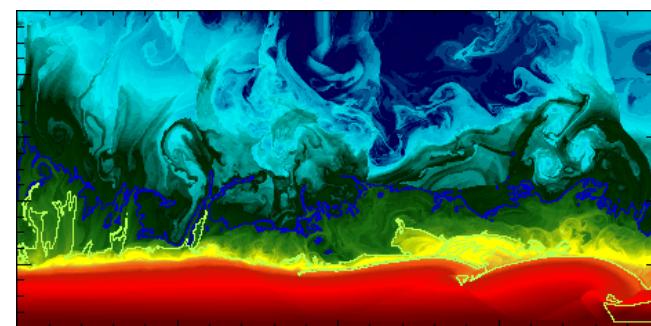
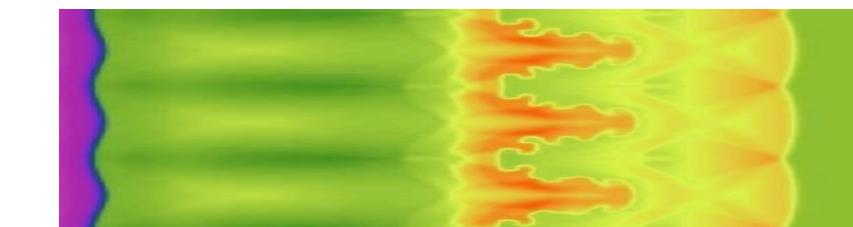
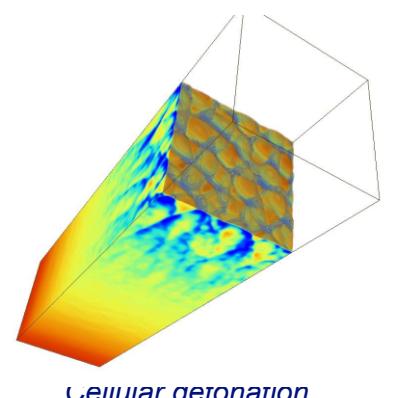
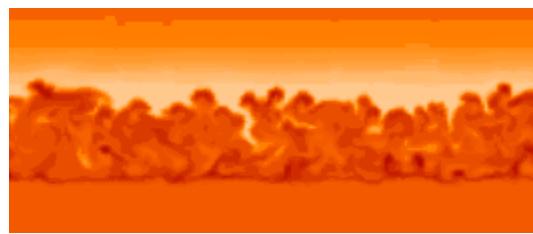
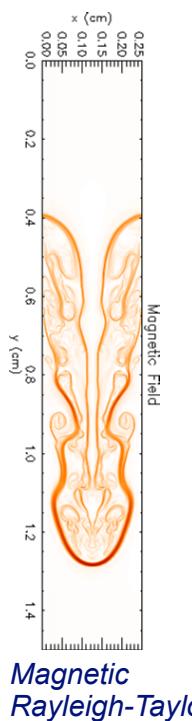
Pinpointing and Quantifying Scalability Bottlenecks



Scalability Analysis Demo

Code:
Simulation:
Platform:
Experiment:
Scaling type:

University of Chicago FLASH
white dwarf detonation
Blue Gene/P
8192 vs. 256 processors
weak



Figures courtesy of FLASH Team, University of Chicago

Scalability Analysis of Flash (Demo)

hpcviewer: FLASH/white dwarf: IBM BG/P, weak 256->8192

Driver_initFlash.F90 local_tree_build.F90

```
206 !----First pass only add lrefine = 1 blocks to tree(s)
207 !----Second pass add the rest of the blocks.
208     Do ipass = 1,2
209
210     lnblocks_old = lnblocks
211     proc = mype
212 !----Loop through all processors
213     Do iproc = 0, nprocs-1
214
215     If (iproc == 0) Then
216         off_proc = .False.
217     Else
```

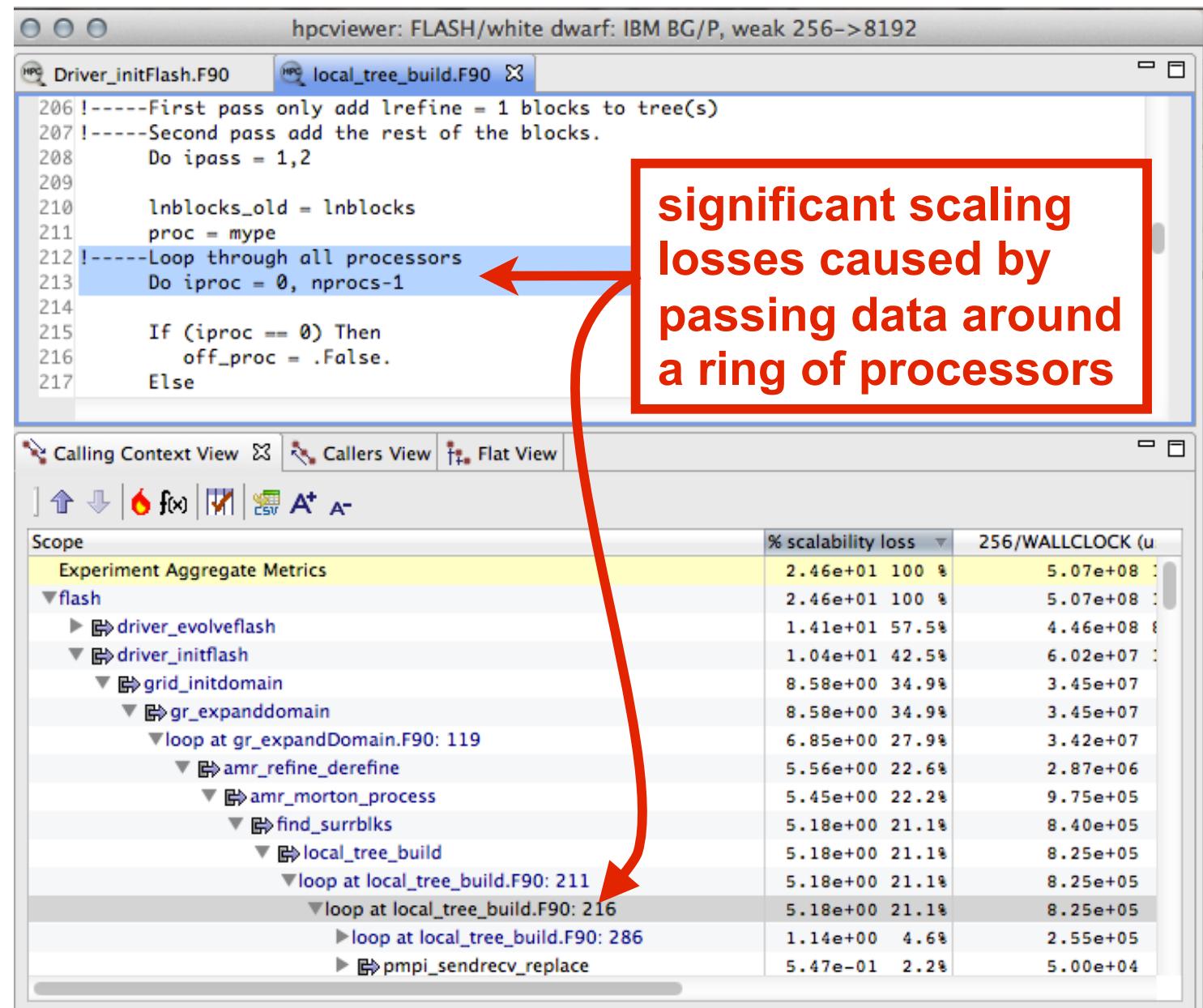
Calling Context View Callers View Flat View

Scope % scalability loss 256/WALLCLOCK (u

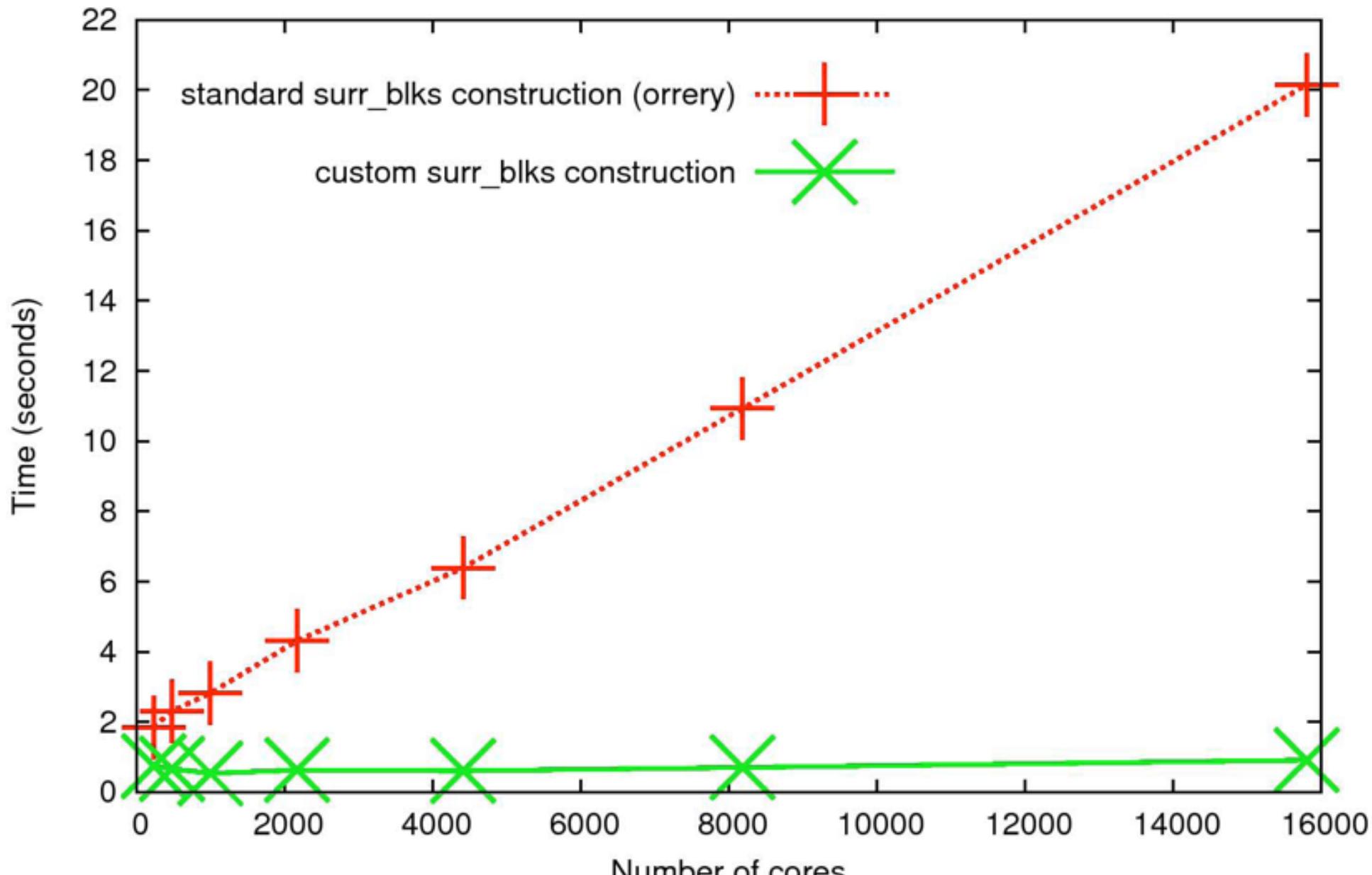
Scope	% scalability loss	256/WALLCLOCK (u
Experiment Aggregate Metrics	2.46e+01 100 %	5.07e+08 1
flash	2.46e+01 100 %	5.07e+08 1
driver_evolvemesh	1.41e+01 57.5%	4.46e+08 8
driver_initmesh	1.04e+01 42.5%	6.02e+07 1
grid_initdomain	8.58e+00 34.9%	3.45e+07
gr_expanddomain	8.58e+00 34.9%	3.45e+07
loop at gr_expandDomain.F90: 119	6.85e+00 27.9%	3.42e+07
amr_refine_derefine	5.56e+00 22.6%	2.87e+06
amr_morton_process	5.45e+00 22.2%	9.75e+05
find_surrlblk	5.18e+00 21.1%	8.40e+05
local_tree_build	5.18e+00 21.1%	8.25e+05
loop at local_tree_build.F90: 211	5.18e+00 21.1%	8.25e+05
loop at local_tree_build.F90: 216	5.18e+00 21.1%	8.25e+05
loop at local_tree_build.F90: 286	1.14e+00 4.6%	2.55e+05
pmpi_sendrecv_replace	5.47e-01 2.2%	5.00e+04

Scalability Analysis

- Difference call path profile from two executions
 - different number of nodes
 - different number of threads
- Pinpoint and quantify scalability bottlenecks within and across nodes



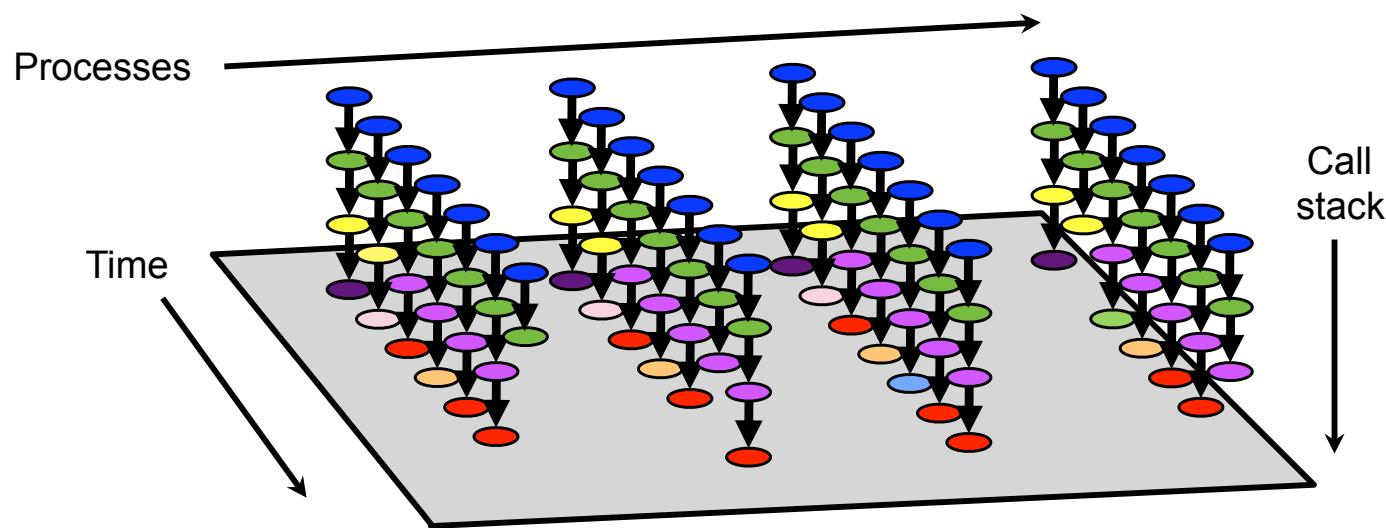
Improved Flash Scaling of AMR Setup



Graph courtesy of Anshu Dubey, U Chicago

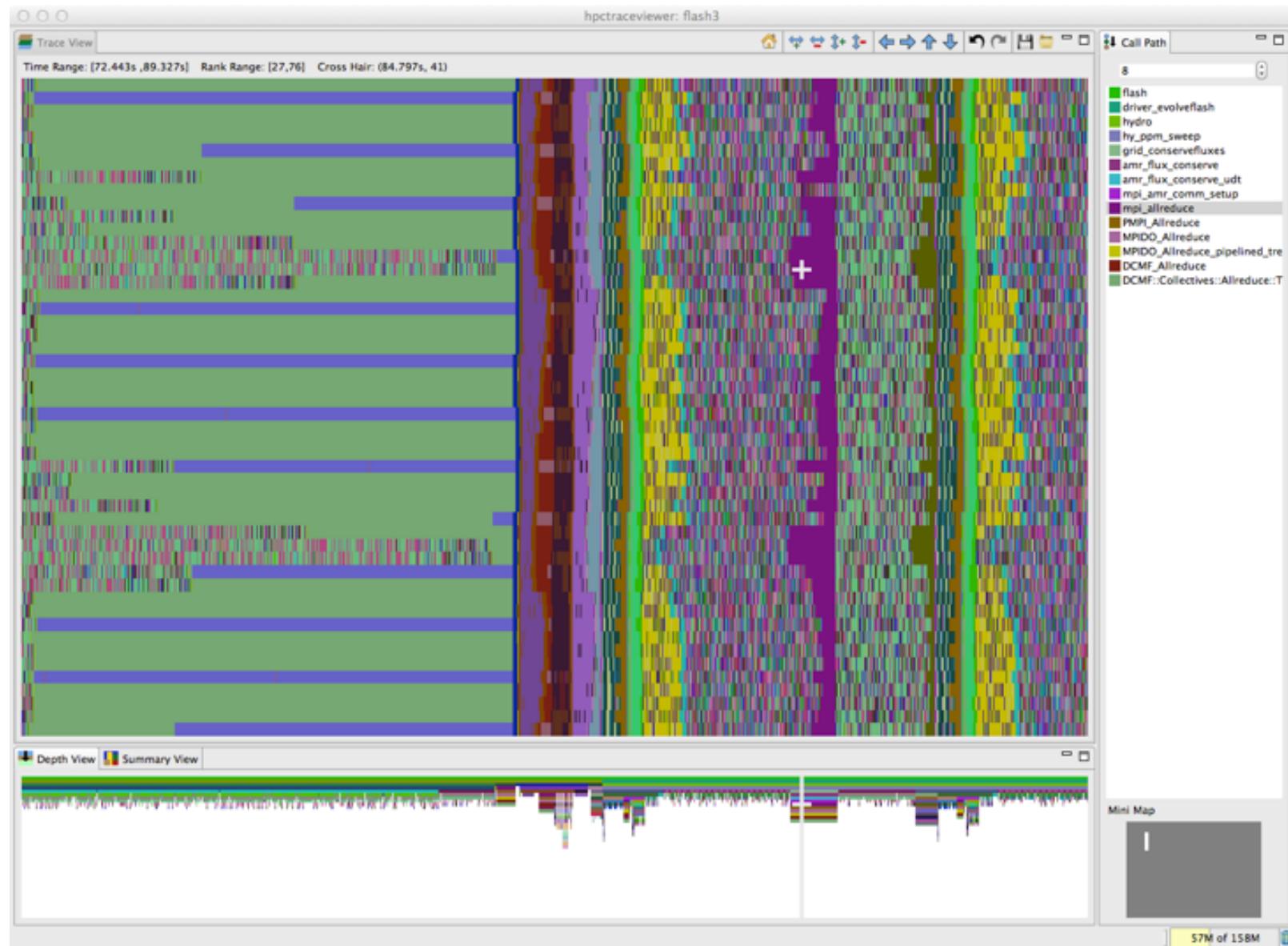
Understanding Temporal Behavior

- Profiling compresses out the temporal dimension
 - temporal patterns, e.g. serialization, are invisible in profiles
- What can we do? Trace call path samples
 - sketch:
 - N times per second, take a call path sample of each thread
 - organize the samples for each thread along a time line
 - view how the execution evolves left to right
 - what do we view?
 - assign each procedure a color; view a depth slice of an execution



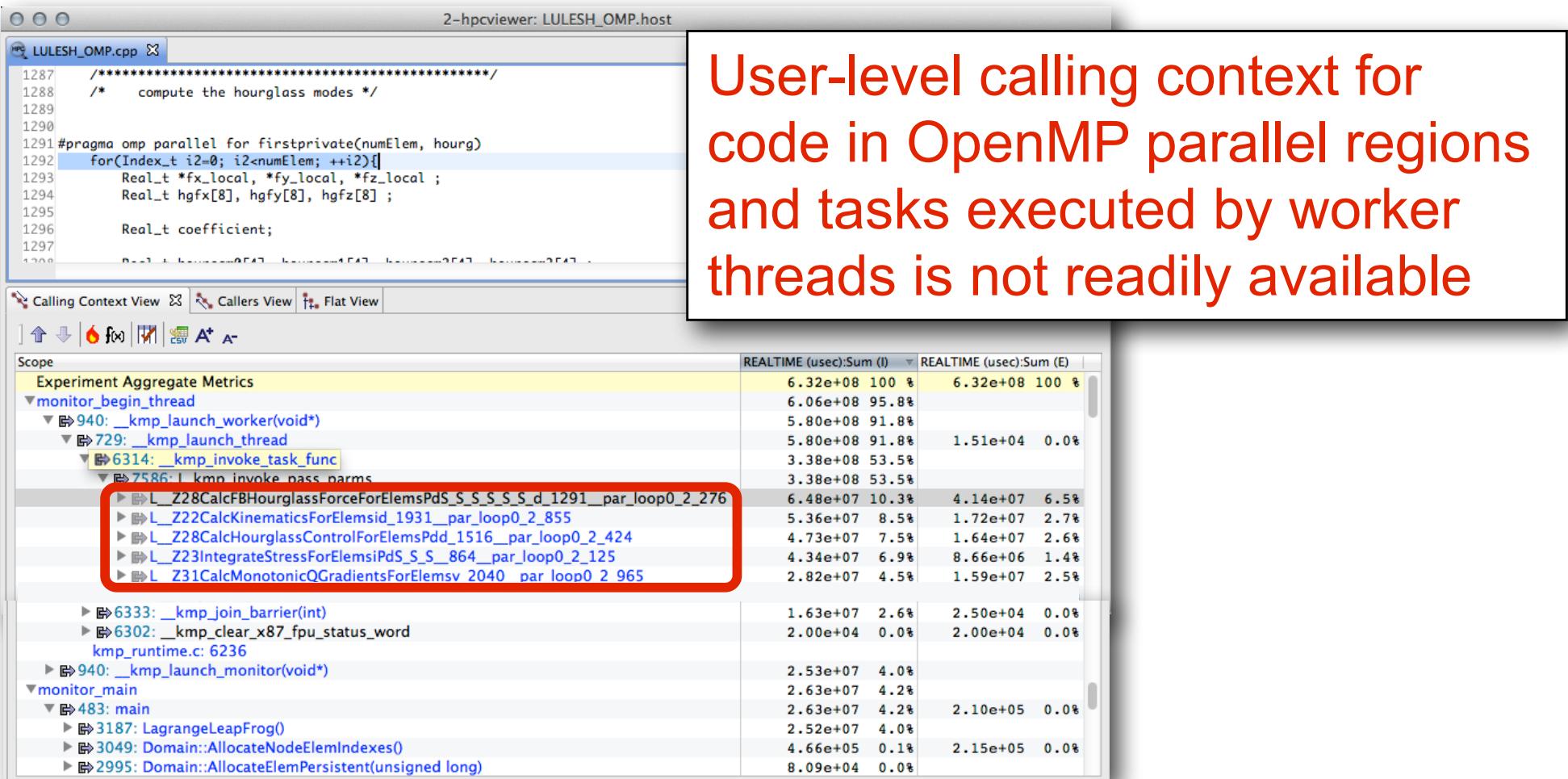
hpctraceviewer: detail of FLASH@256PE

Time-centric analysis: load imbalance among threads appears as different lengths of colored bands along the x axis



OpenMP: A Challenge for Tools

- Large gap between threaded programming models and their implementations



User-level calling context for code in OpenMP parallel regions and tasks executed by worker threads is not readily available

- Runtime support is necessary for tools to bridge the gap

Challenges for OpenMP Node Programs

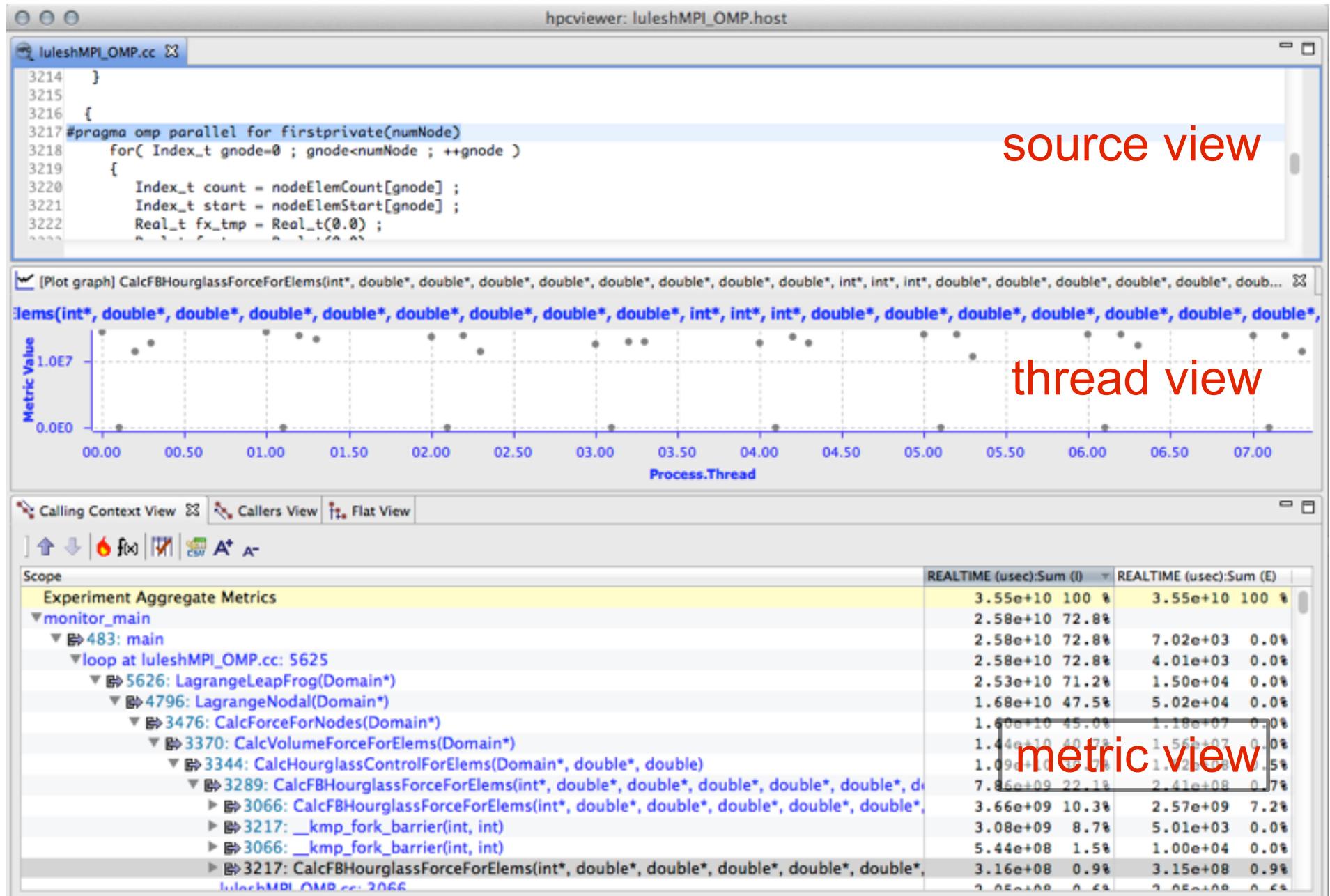
- Tools provide implementation-level view of OpenMP threads
 - asymmetric threads
 - master thread
 - worker thread
 - run-time frames are interspersed with user code
- Hard to understand causes of idleness
 - long serial sections
 - load imbalance in parallel regions
 - waiting for critical sections or locks

OMPT: An OpenMP Tools API

- **Goal: a standardized tool interface for OpenMP**
 - prerequisite for portable tools
 - missing piece of the OpenMP language standard
- **Design objectives**
 - enable tools to measure and attribute costs to application source and runtime system
 - support low-overhead tools based on asynchronous sampling
 - attribute to user-level calling contexts
 - associate a thread's activity at any point with a descriptive state
 - minimize overhead if OMPT interface is not in use
 - features that may increase overhead are optional
 - define interface for trace-based performance tools
 - don't impose an unreasonable development burden
 - runtime implementers
 - tool developers

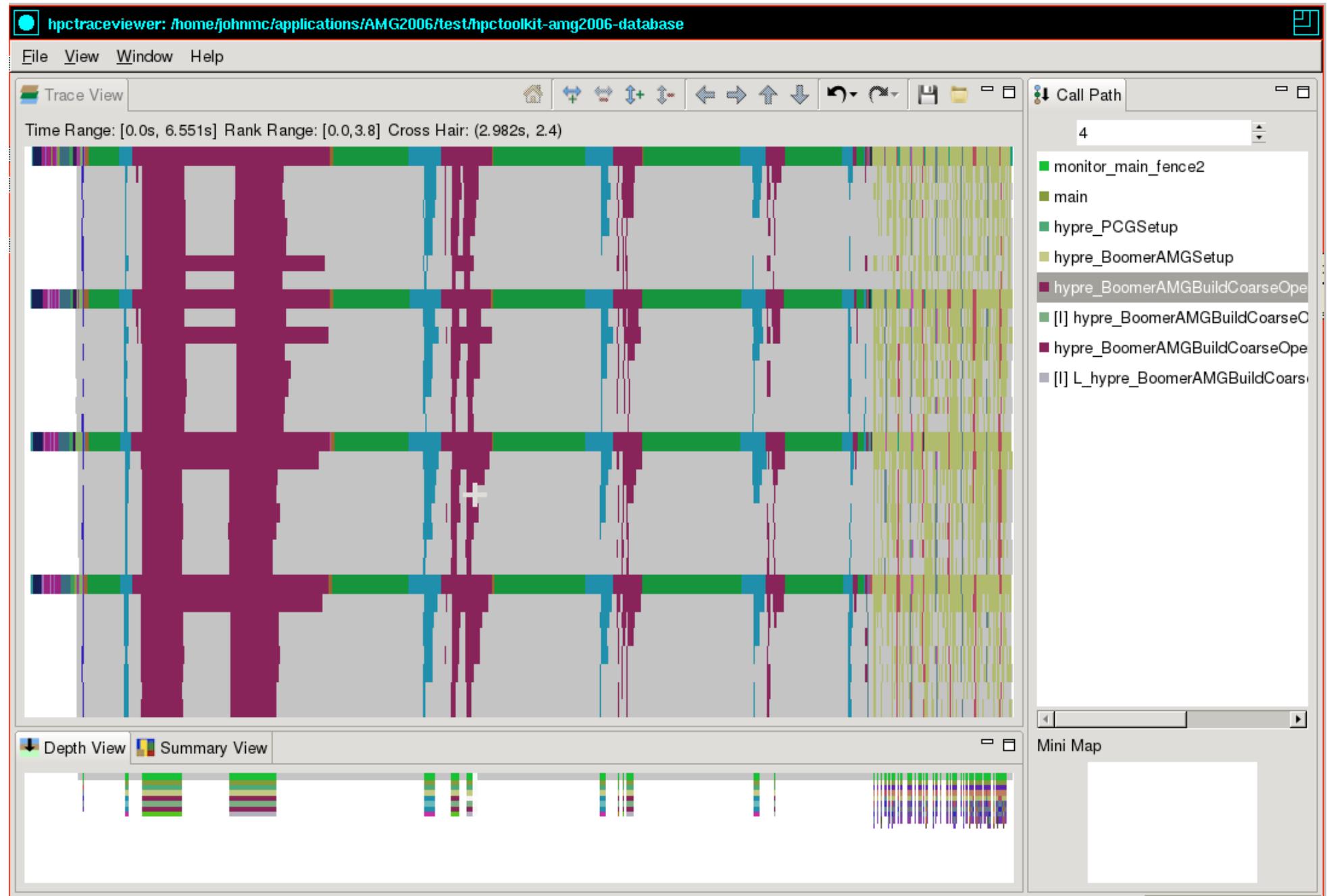
Integrated View of MPI+OpenMP with OMPT

LLNL's IuleshMPI_OMP (8 MPI x 3 OMP), 30, REALTIME@1000



2 18-core Haswell
4 MPI ranks
6+3 threads per rank

Case Study: AMG2006



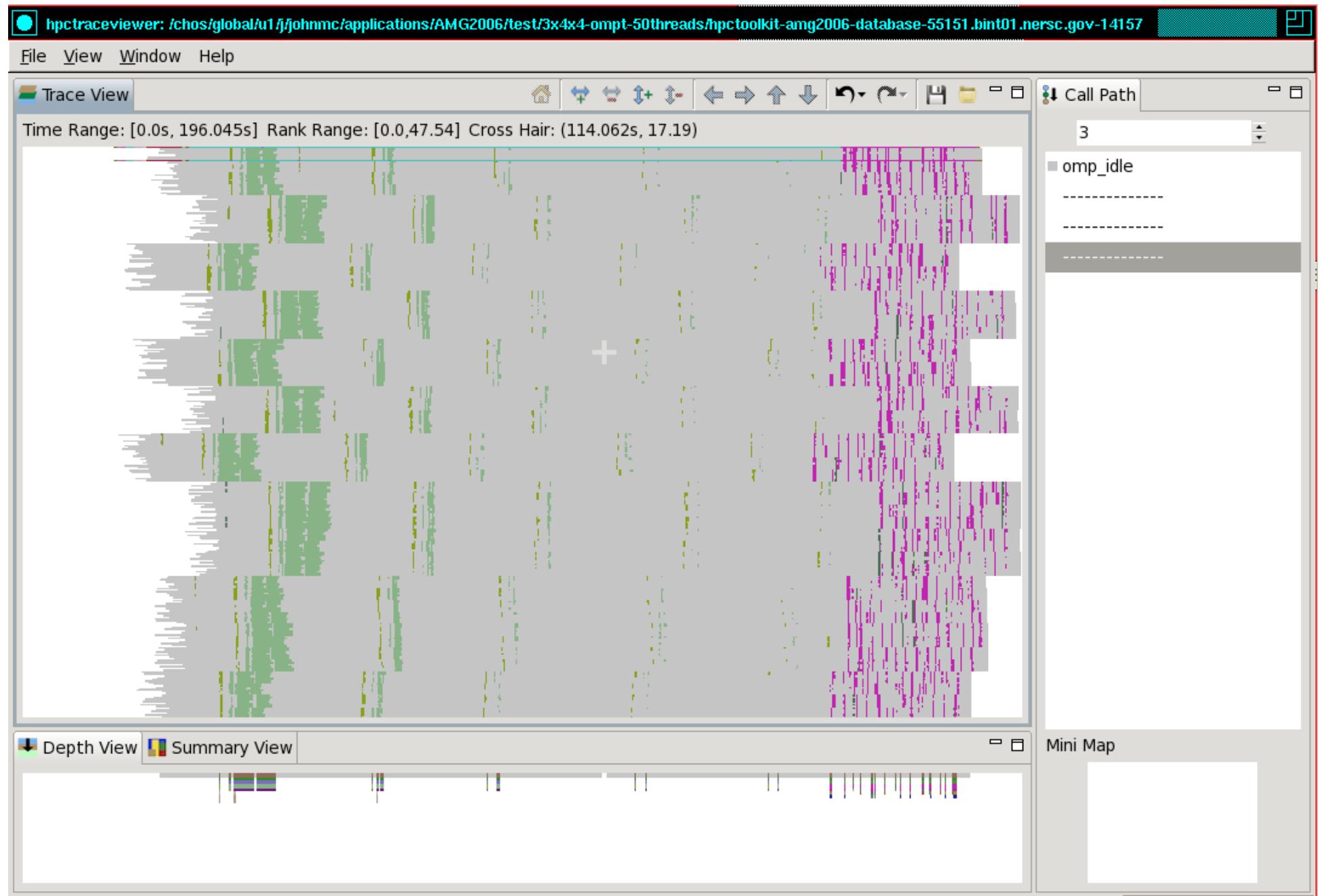
12 nodes on Babbage@NERSC

24 Xeon Phi

48 MPI ranks

50+5 threads per rank

Case Study: AMG2006



12 nodes on Babbage@NERSC

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48 MPI ranks

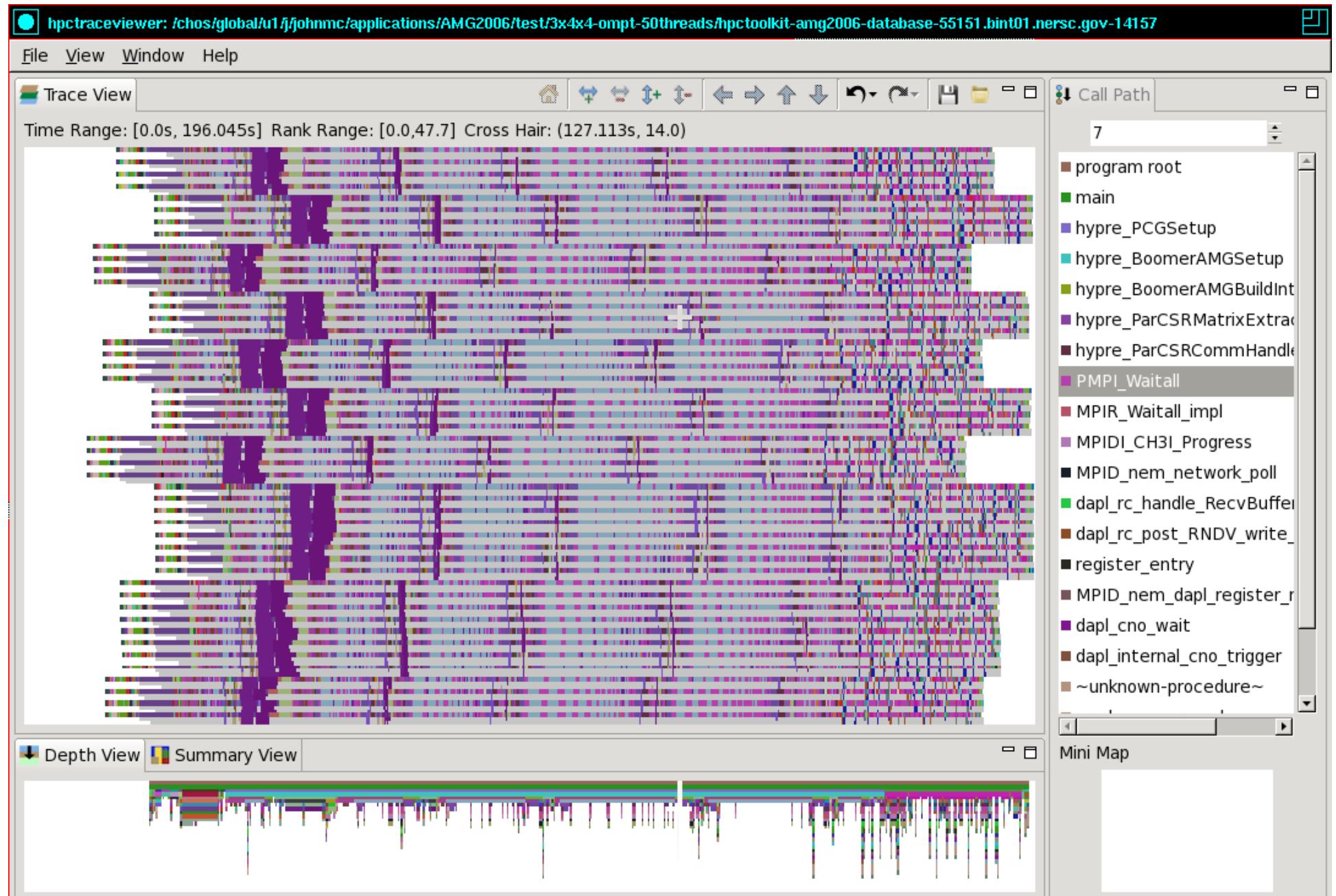
50+5 threads per rank

Case Study: AMG2006

Slice

Thread 0 from each MPI rank

First two OpenMP workers



Blame-shifting: Analyze Thread Performance

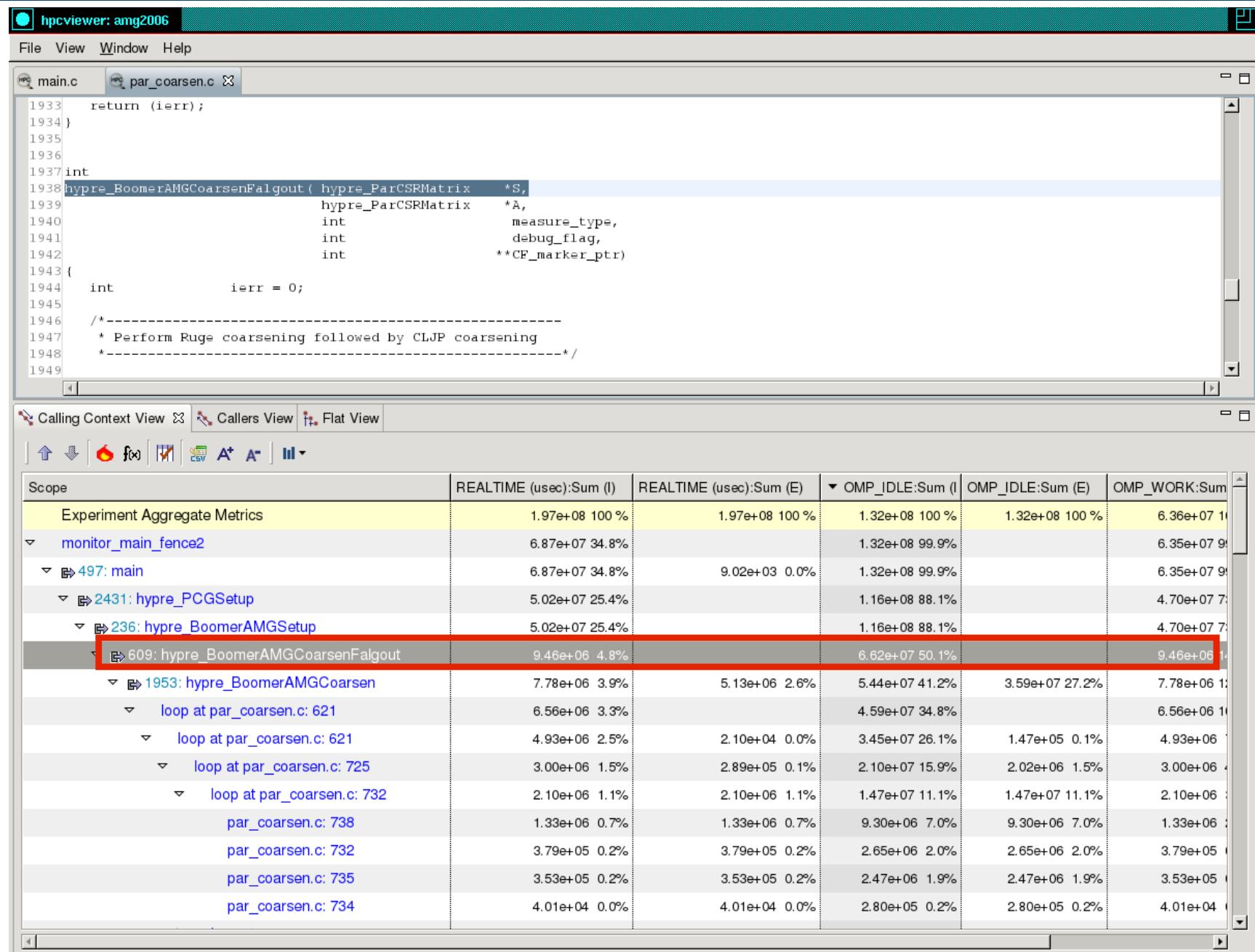
	Problem	Approach
Undirected Blame Shifting ^{1,3}	A thread is idle waiting for work	Apportion blame among working threads for not shedding enough parallelism to keep all threads busy
Directed Blame Shifting ^{2,3}	A thread is idle waiting for a mutex	Blame the thread holding the mutex for idleness of threads waiting for the mutex

¹Tallent & Mellor-Crummey: PPoPP 2009

²Tallent, Mellor-Crummey, Porterfield: PPoPP 2010

³Liu, Mellor-Crummey, Fagan: ICS 2013

Blame Shifting: Idleness in AMG2006



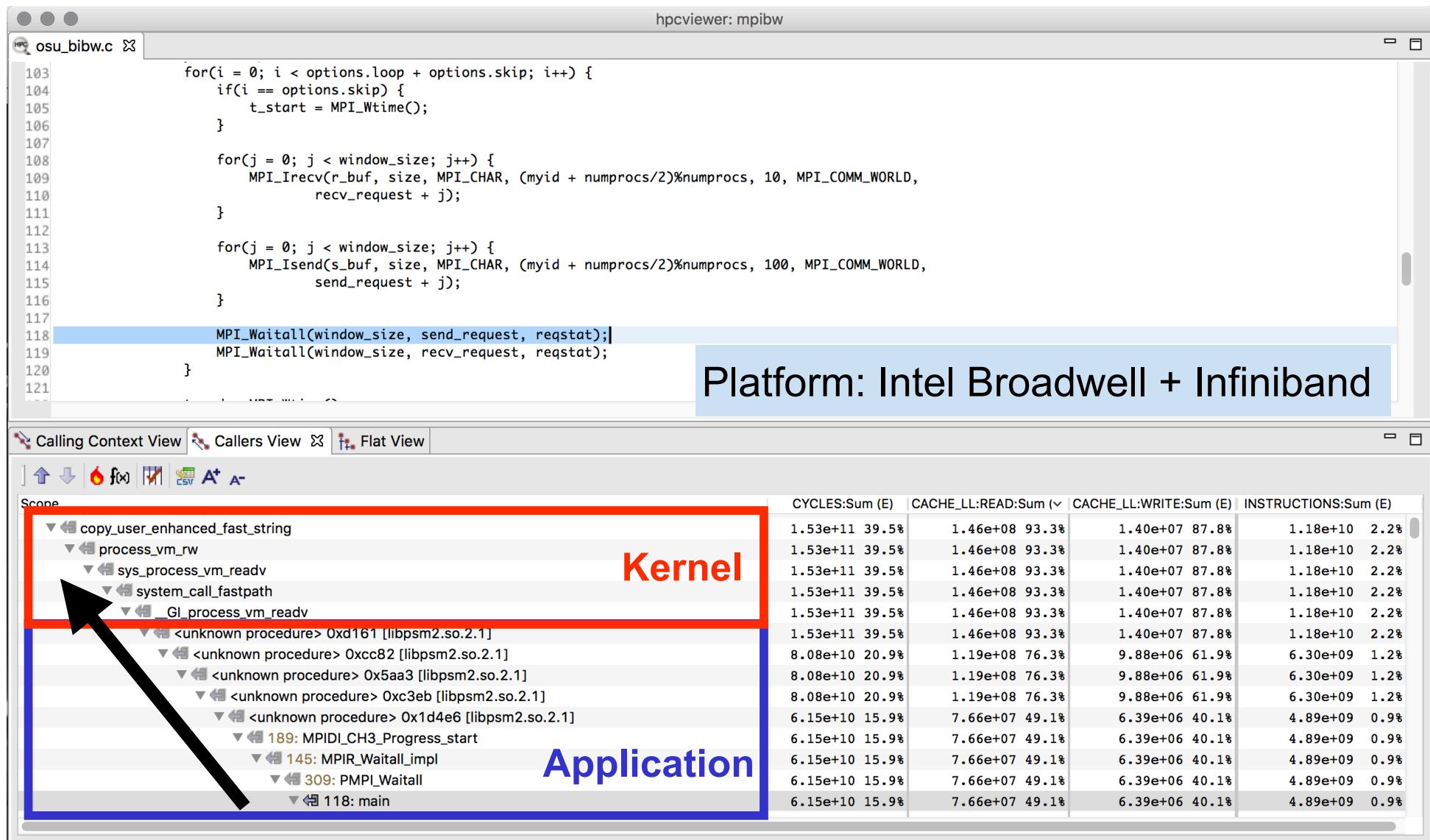
OpenMP Tool API Status

- Currently HPCToolkit supports OMPT interface based on OpenMP TR2 (April 2014)
- Migrating to emerging OpenMP 5.0 (preview, Nov 2016)
- OMPT prototype implementations
 - LLVM (current: OpenMP 5)
 - interoperable with GNU, Intel compilers
 - IBM LOMP (currently targets OpenMP 5)
- Ongoing work
 - refining OpenMP 5.0 definition of OMPT
 - refining OpenMP 5.0 OMPT support in LLVM
 - refining HPCToolkit OMPT to match emerging standard

Emerging Capabilities in Brief

Monitoring Application + Kernel

Sampling call stacks into the kernel



Monitoring Accelerated OpenMP 5

Sampling calling contexts spanning CPU + GPU

2-hpcviewer: lulesh2.0

lulesh.cc lulesh.h

```
2620
2621
2622
2623 {
2624
2625
2626 # pragma omp target teams num_teams(TEAMS) thread_limit(THREADS) if (USE_GPU == 1)
2627 # pragma omp distribute parallel for
2628 for (Index_t i=0; i<numElem; ++i) {
2629     Index_t elem = i;
2630     Index_t rep = elemRep[elem];
2631     Real_t e_old, delvc, p_old, q_old, qq_old, ql_old;
2632     Real_t p_new, q_new, e_new;
2633     Real_t work, compression, compHalfStep, bvc, pbvc, pHalfStep;
2634     Real_t vchalf ;
2635     const Real_t c1s = Real_t(2.0) / Real_t(3.0) ;
2636     Real_t vhalf ;
2637     Real_t ssc ;
2638     const Real_t sixth = Real_t(1.0) / Real_t(6.0) ;
```

Calling Context View Callers View Flat View

Scope

Experiment Aggregate Metrics

<program root>

- 500: main
 - loop at lulesh.cc: 3231
 - 3225: LagrangeLeapFrog(Domain&)
 - 3056: LagrangeElements(Domain&, int)
 - 2864: ApplyMaterialPropertiesForElems(Domain&, double*)
 - 2846: EvalEOSForElems(Domain&, double*)
 - 2626: <unknown procedure>
 - \$_omp_outlined\$_debug\$_29
 - lulesh.cc: 2803
 - lulesh.cc: 2767
 - lulesh.cc: 2725

GPU Instructions

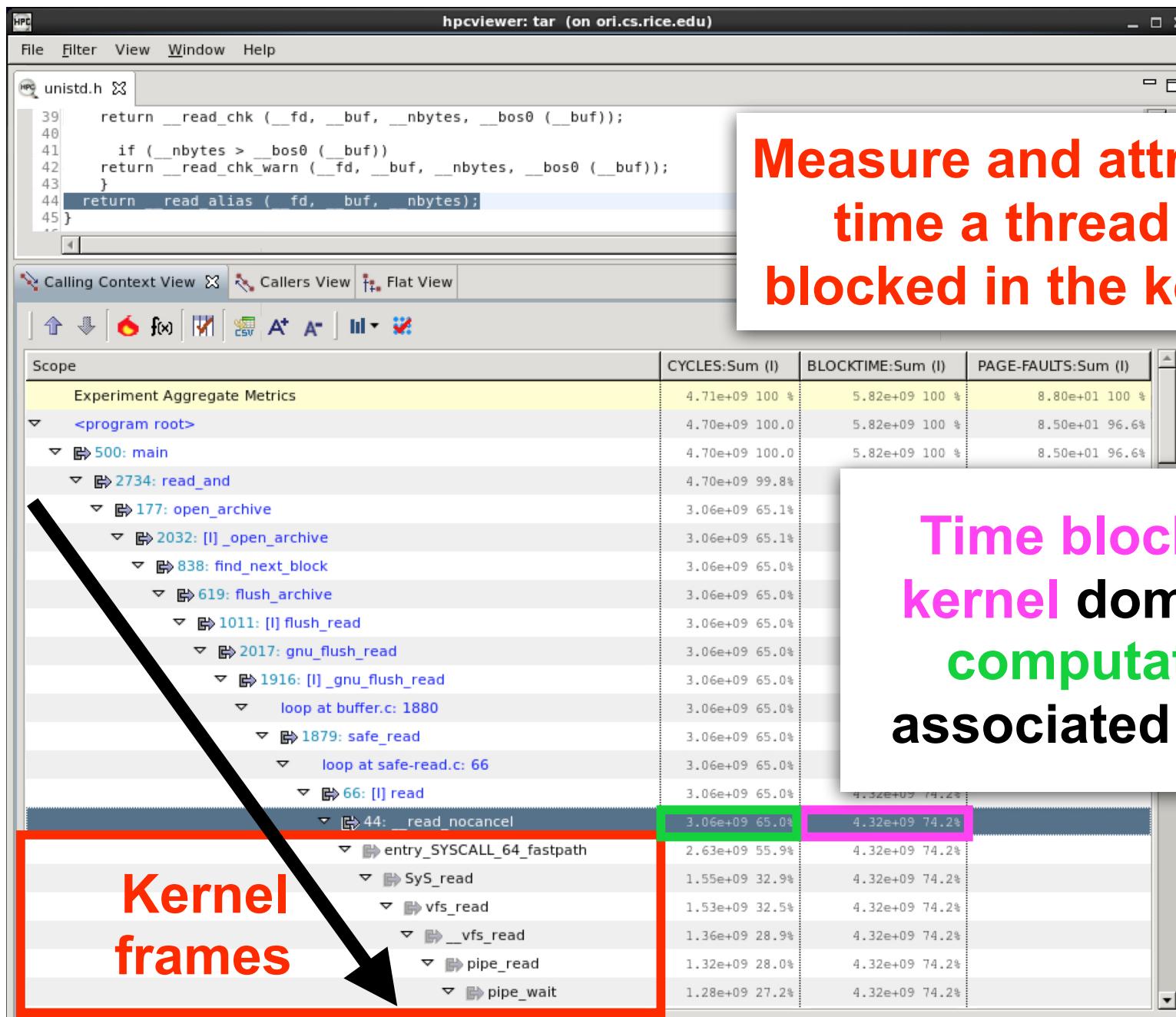
GPU_ISAMP:Sum (I)	STL_SYNC:Sum (I)	STL_EXC_DEP:Sum (I)	STL_MEM_DEP:Sum (I)	STL_NONE:Sum (I)
2.38e+07 100	1.00e+07 100 %	6.48e+06 100 %	6.44e+06 100 %	4.24e+05 100 %
2.38e+07 100	1.00e+07 100 %	6.48e+06 100 %	6.44e+06 100 %	4.24e+05 100 %
2.38e+07 100	1.00e+07 100 %	6.48e+06 100 %	6.44e+06 100 %	4.24e+05 100 %
2.38e+07 100	1.00e+07 100 %	6.48e+06 100 %	6.44e+06 100 %	4.24e+05 100 %
2.38e+07 100	1.00e+07 100 %	6.48e+06 100 %	6.44e+06 100 %	4.24e+05 100 %
2.38e+07 100	1.00e+07 100 %	6.48e+06 100 %	6.44e+06 100 %	4.24e+05 100 %
1.19e+07 50.1	5.19e+06 51.8%	3.42e+06 52.8%	2.86e+06 44.5%	2.21e+05 52.1%
6.34e+06 26.6	2.91e+06 29.1%	1.97e+06 30.4%	1.21e+06 18.8%	1.25e+05 29.5%
6.34e+06 26.6	2.91e+06 29.1%	1.97e+06 30.4%	1.21e+06 18.8%	1.25e+05 29.5%
6.34e+06 26.6	2.91e+06 29.1%	1.97e+06 30.4%	1.21e+06 18.8%	1.25e+05 29.5%
2.71e+06 11.4		1.57e+06 24.2%	9.69e+05 15.0%	9.80e+04 23.1%
1.60e+05 0.7		1.03e+05 1.6%	4.78e+04 0.7%	5.92e+03 1.4%
1.59e+05 0.7		1.02e+05 1.6%	4.79e+04 0.7%	5.92e+03 1.4%
1.59e+05 0.7		1.02e+05 1.6%	4.77e+04 0.7%	6.01e+03 1.4%

Host

GPU



Measuring Thread Blocking



Measure and attribute time a thread is blocked in the kernel

Time blocked in the kernel dominates the computation time associated with reads

Kernel frames

Other Ongoing Work and Future Plans

- Other ongoing work
 - **data-centric analysis: associate costs with variables**
 - analysis and attribution of performance to optimized code
 - **adding OpenMP parallelism to hpcprof-mpi to accelerate data analysis**
 - **adding OpenMP parallelism to hpcstruct to accelerate binary analysis**
 - **automated analysis to deliver performance insights**
- Future plans
 - **support top-down analysis methods using hardware counters**
 - **resource-centric performance analysis**
 - within and across nodes
 - **scale measurement and analysis for exascale**

Status

- New binary analyzer for better attribution of performance to source code merged into master this week
- Resolve conflict between Linux perf_events and Cray PAPI module
- Investigate issue measuring counter events related to SIMD performance
- Attribute kernel time to <vmlinux> if kernel symbols are not available
- Cherry-pick OMPT support for CPU and make it available
- We will update HPCToolkit modules on all ALCF systems once these issues are resolved
- We will email participants when new HPCToolkit installations are available

HPCToolkit at ALCF

- ALCF systems (**vesta, cetus**)
 - BG/Q: in your **.soft** file, add the following line
 - **+hpctoolkit-devel**
(this package is always the most up-to-date)
 - Theta
 - **module load hpctoolkit**
- Man pages
 - available but not provided in module on theta
- ALCF guide to HPCToolkit
 - <http://www.alcf.anl.gov/user-guides/hpctoolkit>
- Download binary packages for HPCToolkit's user interfaces on your laptop
 - <http://hpctoolkit.org/download/hpcviewer>

Detailed HPCToolkit Documentation

<http://hpctoolkit.org/documentation.html>

- **Comprehensive user manual:**

<http://hpctoolkit.org/manual/HPCToolkit-users-manual.pdf>

- **Quick start guide**

- essential overview that almost fits on one page

- **Using HPCToolkit with statically linked programs**

- a guide for using hpctoolkit on BG/Q and Cray platforms

- **The hpcviewer and hpctraceviewer user interfaces**

- **Effective strategies for analyzing program performance with HPCToolkit**

- analyzing scalability, waste, multicore performance ...

- **HPCToolkit and MPI**

- **HPCToolkit Troubleshooting**

- why don't I have any source code in the viewer?

- hpcviewer isn't working well over the network ... what can I do?

- **Installation guide**

Advice for Using HPCToolkit

Using HPCToolkit

- Add hpctoolkit's bin directory to your path using softenv
- Adjust your compiler flags (if you want full attribution to src)
 - add -g flag after any optimization flags
- Add hpmlink as a prefix to your Makefile's link line
 - e.g. `hpmlink mpixlf -o myapp foo.o ... lib.a -lm ...`
- See what sampling triggers are available on BG/Q
 - use hpmlink to link your executable
 - launch executable with environment variable `HPCRUN_EVENT_LIST=LIST`
 - you can launch this on 1 core of 1 node
 - no need to provide arguments or input files for your program
they will be ignored

Collecting Performance Data on BG/Q

- Collecting traces on BG/Q
 - set environment variable `HPCRUN_TRACE=1`
 - use `WALLCLOCK` or `PAPI_TOT_CYC` as one of your sample sources when collecting a trace
- Launching your job on BG/Q using hpctoolkit
 - `qsub -A ... -t 10 -n 1024 --mode c1 --proccount 16384 \ --cwd `pwd` \ --env OMP_NUM_THREADS=2:\ HPCRUN_EVENT_LIST=WALLCLOCK@5000:\ HPCRUN_TRACE=1\ your_executable`

Monitoring Large Executions

- Collecting performance data on every node is typically not necessary
- Can improve scalability of data collection by recording data for only a fraction of processes
 - set environment variable `HPCRUN_PROCESS_FRACTION`
 - e.g. collect data for 10% of your processes
 - set environment variable `HPCRUN_PROCESS_FRACTION=0.10`

Digesting your Performance Data

- Use hpcstruct to reconstruct program structure
 - e.g. `hpcstruct your_app`
 - creates `your_app.hpcstruct`
- Correlate measurements to source code with hpcprof and hpcprof-mpi
 - run hpcprof on the front-end to analyze data from small runs
 - run hpcprof-mpi on the compute nodes to analyze data from lots of nodes/threads in parallel
 - notes
 - much faster to do this on an `x86_64` vis cluster (cooley) than on BG/Q
 - avoid expensive per-thread profiles with `--metric-db no`
- Digesting performance data in parallel with hpcprof-mpi
 - `qsub -A ... -t 20 -n 32 --mode c1 --proccount 32 --cwd `pwd` \ /projects/Tools/hpctoolkit/pkgs-vesta/hpctoolkit/bin/hpcprof-mpi \ -S your_app.hpcstruct \ -I /path/to/your_app/src/+ \ hpctoolkit-your_app-measurements.jobid`
- Hint: you can run hpcprof-mpi on the `x86_64` vis cluster (cooley)

Analysis and Visualization

- Use **hpcviewer** to open resulting database
 - warning: first time you graph any data, it will pause to combine info from all threads into one file
- Use **hpctraceviewer** to explore traces
 - warning: first time you open a trace database, the viewer will pause to combine info from all threads into one file
- Try our user interfaces before collecting your own data
 - example performance data
<http://hpctoolkit.org/examples.html>

Installing HPCToolkit GUIs on your Laptop

- See <http://hpctoolkit.org/download/hpcviewer>
- Download the latest for your laptop (Linux, Mac, Windows)
 - **hpctraceviewer**
 - **hpcviewer**

A Note for Mac Users

When installing HPCToolkit GUIs on your Mac laptop, don't simply download and double click on the zip file and have Finder unpack them. Follow the Terminal-based installation directions on the website to avoid interference by Mac Security.